

# Temperature Fluctuation Scaling in Reacting Boundary Layers

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## Abstract

The direct numerical simulation (DNS) data of a turbulent, reacting boundary layer is used to study the turbulence-chemistry interaction and the scaling of the temperature fluctuations. We find that there is a feedback between the turbulence and the chemical reactions. Temperature fluctuations increase the reaction rates. Endothermic reactions reduce the magnitude of the temperature fluctuations. However, the turbulent boundary layer is self-sustained and the magnitude of the temperature fluctuations is maintained. Exothermic reactions increase the magnitude of the temperature fluctuations. The reactions cause localized compressions and expansions that feed the turbulent kinetic energy. The evolution equations for the turbulent energy show that the feedback takes place through the transport and production terms. The data reveals a physically consistent relation between the temperature variance and the mean flow parameters. These results are consistent with those previously found in reacting isotropic turbulence.<sup>1,2</sup>

## Introduction

The boundary layers that are formed on hypersonic vehicles are hot, chemically reacting, and turbulent. Currently, the boundary layer on realistic hypersonic vehicles is simulated either assuming that the boundary layer is laminar or using simple models that have not been calibrated for hypersonic applications. Generally, the calibration of turbulent models has been done using DNS databases of incompressible flows or using perfect gas wind tunnel data. If we were able to perform more accurate simulations of hypersonic flows, we may find a different chemical composition of the gas, and different heating-rates than those that are currently predicted.

In the flows of interest the magnitude of the temperature fluctuations is very large due to the high energy content that is present. Furthermore, the chemical reaction is a highly non-linear function of the temperature. Therefore, temperature fluctuations may result in large variations in the reaction rates. In this paper we study the turbulence-chemistry interaction in a turbulent boundary layer and seek a scaling of the temperature fluctuations based on the resolved mean flow

variables. The aim is to devise a model for the temperature fluctuations that can be used in the context of Reynolds-averaged Navier-Stokes or large-eddy simulations to predict accurate heating-rates and product formation.

Following our previous work,<sup>3</sup> we use the DNS database of a boundary layer at  $Re_\theta = 7000$ , edge-conditions of  $M_e = 4.0$ ,  $\rho_e = 0.5 \text{ kg/m}^3$ ,  $T_e = 5000 \text{ K}$ , and wall-temperature  $T_w = 5000 \text{ K}$ . These conditions represent the boundary layer on a 26° wedge at a Mach number of 20 and 20 km altitude. We use a single model reaction,  $S1 + M \rightleftharpoons S2 + M$ , where species S1 and S2 have the same molecular weight and number of degrees of freedom. In this way, the gas constant is not a function of the chemical composition of the gas and changes in pressure are only caused by density and temperature variations. The reaction rates correspond to oxygen dissociation, and S1 and S2 represent molecules and atoms, respectively. Thus, production of species S1 indicates an exothermic reaction. The reaction rate and equilibrium constant expressions are taken from Gupta *et al.*<sup>4</sup>

The paper is organized as follows. We first present a review of our previous work by introducing the non-dimensional parameters that govern the turbulence-chemistry interaction and the scaling functions that were found using DNS data of isotropic turbulence at conditions typical of hypersonic boundary layers. In a turbulent boundary layer, the energy transfer mechanisms are more complex than those found in isotropic turbulence. Thus, we present the temporal evolution equations for the turbulent kinetic energy and the variance of the temperature. These equations are used in the analysis of the turbulence-chemistry interaction. The results are divided in two sections. First, we present the characteristics of the mean flow and the effect of turbulent fluctuations on the mean flow motion. We then discuss the turbulent energy transfer and the scaling of the temperature fluctuations. Conclusions are given in the last section.

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<b>Report Documentation Page</b>			Form Approved OMB No. 0704-0188		
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1. REPORT DATE <b>JUN 2001</b>	2. REPORT TYPE	3. DATES COVERED <b>00-00-2001 to 00-00-2001</b>			
4. TITLE AND SUBTITLE <b>Temperature Fluctuation Scaling in Reacting Boundary Layers</b>			5a. CONTRACT NUMBER		
			5b. GRANT NUMBER		
			5c. PROGRAM ELEMENT NUMBER		
6. AUTHOR(S)			5d. PROJECT NUMBER		
			5e. TASK NUMBER		
			5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) <b>University of Minnesota, Department of Aerospace Engineering and Mechanics, 110 Union St. SE, Minneapolis, MN, 55455</b>			8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)			10. SPONSOR/MONITOR'S ACRONYM(S)		
			11. SPONSOR/MONITOR'S REPORT NUMBER(S)		
12. DISTRIBUTION/AVAILABILITY STATEMENT <b>Approved for public release; distribution unlimited</b>					
13. SUPPLEMENTARY NOTES <b>AIAA Paper No. 01-2717, 31st AIAA Fluids Dynamics Conference, Anaheim, CA, June 2001. Also in Annual Research Briefs, Center for Turbulence Research, NASA Ames/Stanford University, 2001.</b>					
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15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT <b>unclassified</b>	b. ABSTRACT <b>unclassified</b>	c. THIS PAGE <b>unclassified</b>	<b>Same as Report (SAR)</b>	<b>8</b>	

## Background

The nondimensional parameters governing the turbulence chemistry interaction are<sup>1</sup> the turbulent Mach number, the Reynolds number, the Damköhler number, and the relative heat release, namely

$$\begin{aligned} M_t &= \frac{q}{a}, & Re_\lambda &= \frac{\rho u' \lambda}{\mu}, \\ Da &= \frac{\tau_t}{\tau_c}, & \overline{\Delta h^\circ} &= - \frac{\Delta h^\circ}{c_v T + \frac{1}{2} q^2}, \end{aligned} \quad (1)$$

where  $q = \langle u'_i u'_i \rangle^{1/2}$  is the rms magnitude of the fluctuation velocity;  $a$  is the speed of sound;  $\tau_t = k/\epsilon$  is the turbulent time scale, where  $k$  and  $\epsilon$  are the turbulent kinetic energy and dissipation, respectively;  $\tau_c = \rho / (\langle w_{S1}^2 \rangle^{1/2} K_{eq})$  is the chemical time scale where  $w$  is the source term, and  $K_{eq}$  is the equilibrium constant;  $\lambda = q \tau_t$  is the characteristic turbulent length scale; and  $\Delta h^\circ$  is the heat of the reaction.

In our previous work,<sup>1,2</sup> we used DNS to perform a fundamental study of isotropic turbulence interacting with finite-rate chemical reactions at conditions typical of a hypersonic boundary layer. We found that the turbulent motion is fed from the energy provided by the exothermic reactions, while the reaction rate is increased by the turbulent temperature fluctuations. This is a feedback process that takes place through the pressure-strain term in the Reynolds stress equation. The feedback is negative for endothermic reactions, resulting in a reduction in the turbulent motion. The DNS database showed that the temperature fluctuations can be expressed as a function of the governing parameters. For endothermic reactions, the temperature fluctuations scale linearly with  $M_t^2$ . Whereas for exothermic reactions, the temperature fluctuations are enhanced and can be expressed as

$$\begin{aligned} T'_{RMS}/\langle T \rangle &= A (\overline{\Delta h^\circ} \lambda/l_E)^B \\ &= A (\overline{\Delta h^\circ} M_t Da)^B \end{aligned} \quad (2)$$

where  $A$  and  $B$  are constants that depend on the specific reaction and  $\lambda$ , also known as the Taylor microscale, represents the distance traveled by a fluid particle moving at the speed of the turbulent intensity. The expansion length  $l_E$  is defined as  $a \tau_c$ , which is the distance traveled by acoustic radiation from the chemistry-induced temperature fluctuations. Therefore,  $\lambda/l_E$  represents the ratio of the characteristic distance traveled by a typical particle of fluid to the characteristic distance traveled by the acoustic radiation.

Another way to understand this ratio of length scales is to consider the variation of the strength of the

chemistry-turbulence interaction. A positive temperature fluctuation increases the reaction rate, making the reaction occur more quickly, which releases more heat, further increasing the temperature. However, the feedback process can be weakened by delocalization of the interaction through turbulent motion and motion generated by the local pressure fluctuations (also caused by the interaction). Therefore, in a simplified case where the reaction rate is held constant, the strength of the interaction varies like  $(u')^2 \frac{1}{u'} \frac{1}{a} = \frac{u'}{a} = M_t$ . In general, the interaction strength also varies with the reaction rate, or in non-dimensional terms, with the Damköhler number. Thus with this argument, we obtain the result shown in eq. (2).

Under the conditions chosen for our calculations of isotropic turbulence,  $\lambda/l_E$  was always less than one. As  $\lambda/l_E$  approaches one,  $T'_{RMS}/\langle T \rangle$  becomes large, indicating a strong turbulence-chemistry interaction. This occurs when the fluid travels a similar distance as the acoustic radiation induced by the temperature fluctuations. If  $\lambda/l_E$  were larger than one, the interaction would be expected to weaken because the turbulent motion would outrun the acoustic waves produced by the interaction, and the feedback process would be diminished. Also, as  $\lambda/l_E$  approaches zero the pressure waves outrun the fluid motion and the interaction is weak. Thus, the interaction weakens when  $\lambda/l_E$  departs from unity. In addition,  $T'_{RMS}/\langle T \rangle$  is affected by the heat released to the flow,<sup>1</sup> and the length ratio must be modulated by  $\overline{\Delta h^\circ}$  to give an appropriate relation for the standard deviation. When  $\lambda/l_E$  is greater than one, we would not expect this fit to be valid because it predicts a further strengthening of the interaction. The Reynolds number did not have a significant effect for the range of conditions that we considered. A more detailed discussion about this scaling for the temperature fluctuations can be found in Martin & Candler.<sup>2</sup>

## Turbulence mechanisms

The chemical reactions act as energy sources within the turbulent boundary layer. Thus, we must address the energy exchange between the turbulence and the chemical reactions. There are four energy exchange mechanisms that take place in turbulent boundary layers: transport, production, dissipation and diffusion of turbulence. The budget equation for the turbulent kinetic energy is

$$\frac{\partial}{\partial t} (\overline{\rho} \tilde{k}) + \tilde{w} \frac{\partial}{\partial z} (\overline{\rho} \tilde{k}) = P_k + T_k + \Pi_t + \Pi_d + \phi_{dif} + \phi_{dis} \quad (3)$$

where

$$\begin{aligned} P_k &= -\overline{\rho u''_i w''} \frac{\partial u''_i}{\partial z}, \\ T_k &= -\frac{1}{2} \frac{\partial}{\partial z} \overline{\rho u''_i u''_i w''}, \\ \Pi_t &= -\frac{\partial}{\partial z} \overline{w'' p'}, \quad \Pi_d = \overline{p' \frac{\partial u''_i}{\partial x_i}}, \\ \phi_{dif} &= \frac{\partial}{\partial z} \overline{u''_i \sigma'_{i2}}, \quad \phi_{dis} = \overline{\sigma'_{ij} \frac{\partial u''_i}{\partial x_j}}, \end{aligned}$$

and  $P_k$  is the production due to the mean gradients,  $T_k$  is the redistribution of turbulent kinetic energy,  $\Pi_t$  is the pressure diffusion, and  $\Pi_d$  is the pressure dilation,  $\phi_{dif}$  is the viscous diffusion,  $\phi_{dis}$  is the viscous dissipation. There are other terms that appear in the equation due to the Favre averaging, however these terms are negligible. Note that  $u'$  and  $u''$  represent fluctuations with respect to the Reynolds and Favre averages of  $u$ , respectively.

To study the turbulent internal energy we use the evolution equation for the temperature variance, which is given by

$$\frac{D\overline{T'^2}}{Dt} = P_T + T_T + \varphi_{vdis} + \varphi_{tdif} + \varphi_{sdif} \quad (4)$$

where

$$\begin{aligned} P_T &= -\frac{2}{c_v} \overline{T'} \sum_s \frac{w_s h_s^\circ}{\rho_s} \\ T_T &= -2(\gamma - 1) \overline{TT'} \frac{\partial u_j}{\partial x_j} \\ \varphi_{vdis} &= \frac{2}{c_v} \frac{\tau_{ij}}{\rho} \frac{\partial u_i}{\partial x_j} T' \\ \varphi_{tdif} &= -\frac{2}{c_v} \frac{T'}{\rho} \frac{\partial q_j}{\partial x_j} \\ \varphi_{sdif} &= -2\gamma \frac{T'}{\rho} \frac{\partial}{\partial x_j} \sum_s \rho D \frac{\partial c_s}{\partial x_j} T \end{aligned}$$

and  $P_T$  is the production of temperature fluctuations due to the chemical reactions and  $h^\circ$  is the heat of formation of species  $s$ ;  $T_T$  is the transport of temperature fluctuations due to the temperature-dilatation correlation;  $\varphi_{vdis}$  represents the viscous dissipation of kinetic energy into internal energy;  $\varphi_{tdif}$  is the diffusion of temperature fluctuations due to heat conduction  $q_j = -\kappa \partial T / \partial x_j$ ; and  $\varphi_{sdif}$  is the redistribution of temperature fluctuations due to the diffusion of species, where  $D$  is the species diffusivity and  $c_s$  is the mass fraction of species  $s$ . The last term,  $\varphi_{sdif}$  is

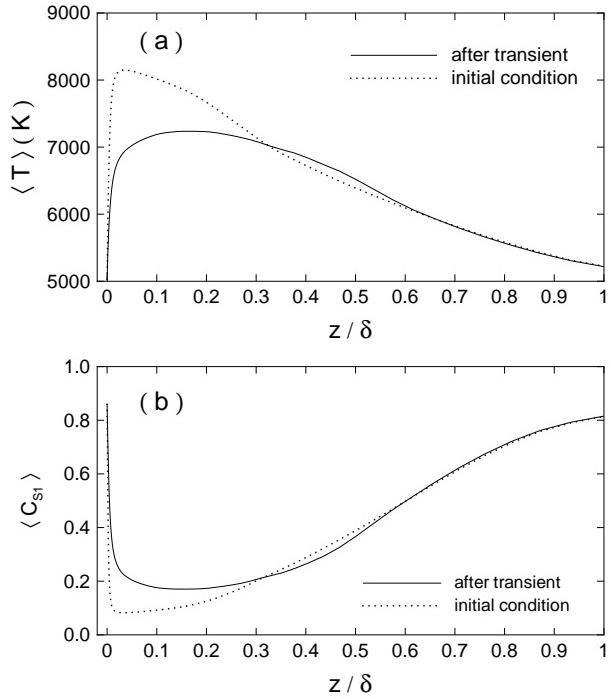


FIGURE 1. Average (a) temperature and (b) mass fraction of species S1.

negligible since for our model reaction the gradients of species S1 and S2 are equal in magnitude and opposite in sign.

### Flow characteristics

The species mass fractions are initialized to their equilibrium values at the averaged temperature. This initial state is not physical. Thus, when we turn on the reactions the flow undergoes a transient. Figure 1a shows the average temperature for the initial condition and after the transient. The gas near the wall is cooled considerably. The temporal evolution equation for the average temperature shows that the mechanisms causing this effect are the chemical source term and the thermal diffusion. Figure 1b, however, shows that the mass fraction of species S1 increases through the transient. Production of S1 indicates exothermic reactions, which would result in an increase of the average temperature. This result can be explained by looking at the budget of the terms in the evolution equation for the density of species S1, which shows that, locally, species S1 diffuses at a faster rate than the source term is destroying it. After the initial transient, the mean flow is in a quasi-equilibrium state. Although the chemical composition in typical hypersonic boundary layers is not in chemical equilibrium, these flow conditions serve to isolate the effect of turbulent fluctuations in the turbulence-chemistry interaction.

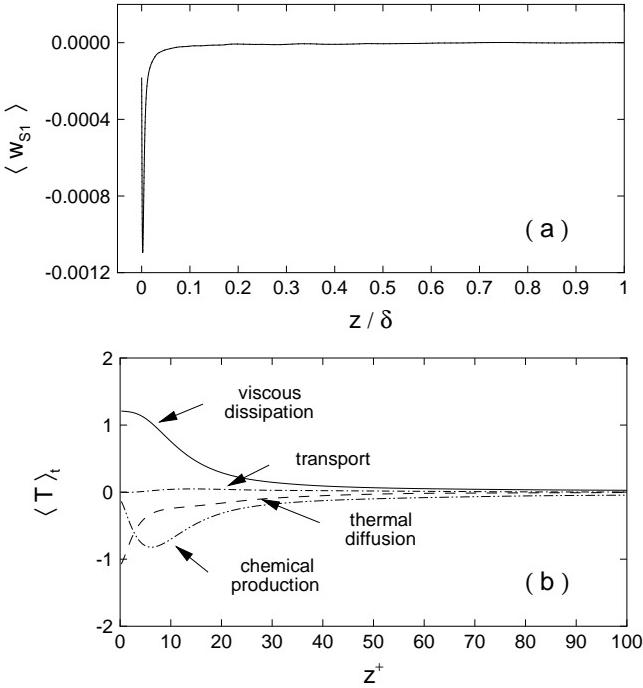


FIGURE 2. (a) Average production of species S1 normalized by  $\rho_w u_\tau / z_\tau$ ; (b) budget for the time evolution of the average temperature normalized by  $u_\tau^3 / cv z_\tau$ .

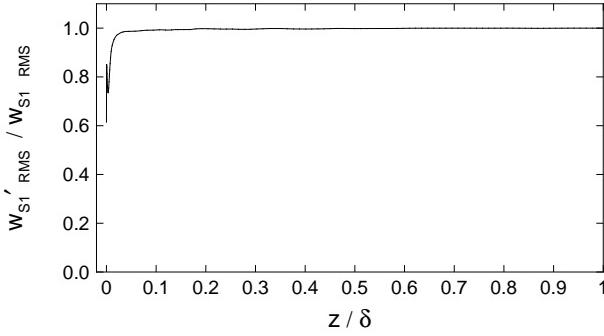


FIGURE 3. Normalized magnitude of the fluctuations in the production of species S1.

Figure 2a shows the average production of S1. There is nearly no net chemical production away from the wall. At the wall  $w_s$  is negative, indicating that destruction of S1 or endothermic reactions are dominant. As mentioned above, the mean flow is in chemical equilibrium, thus the average temperature should not decrease due to the endothermic reactions. Figure 2b shows the budget for the terms in the evolution equation for  $\langle T \rangle_t$ . This equation is similar to the equation for  $\langle T' T' \rangle_t$  but without the factors of  $2T'$  in the terms on the right-hand side of eq. (4). We observe that the effect of the endothermic reactions is to decrease

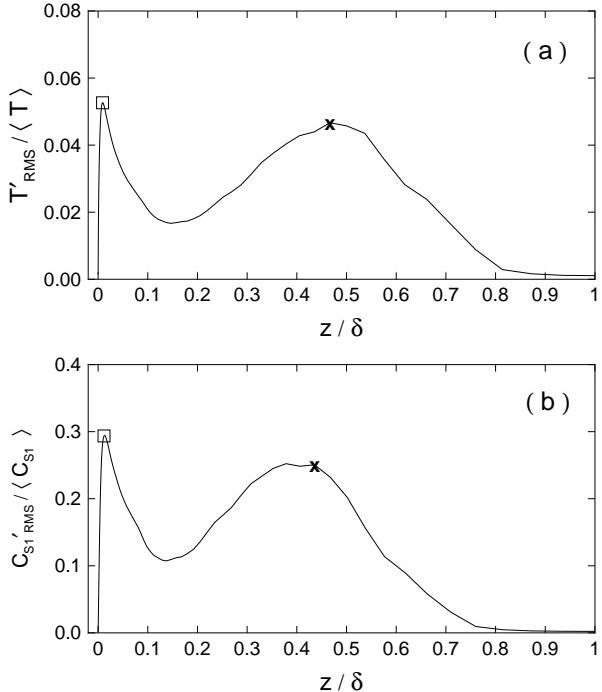


FIGURE 4. Normalized magnitude of the fluctuations in (a) temperature and (b) mass fraction of species S1.

the temperature. Also the effect of the thermal diffusion is to cool the gas near the wall. However, these mechanisms are balanced by the large dissipation of kinetic energy into heat, which is represented by the viscous dissipation.

We now consider the effect of the turbulent fluctuations in the mean flow. Figure 3 shows the rms of the fluctuating source term normalized by its absolute magnitude. The magnitude of the fluctuations are higher than 60% of the average production at the wall and 100% elsewhere, indicating that the production of species is mainly due to fluctuations in the source term. The temperature fluctuations drive the chemical source term and since the mean flow is in equilibrium, no effect is observed in the average chemical composition of the gas, namely  $\langle c_{S1} \rangle$  equals its equilibrium value based on the averaged temperature. However, we should be able to observe an effect on the magnitude of the fluctuating  $c_{S1}$ . Figure 4a shows the magnitude of the temperature fluctuations after the initial transient. The maximum is roughly 5% of the average and takes place in the viscous sublayer. A second peak of nearly the same magnitude develops in the logarithmic region. These locations are marked with symbols. For a given temperature there is a corresponding equilibrium composition of the gas.<sup>4</sup> Table 1 gives the values of  $c_{S1}$  evaluated at  $\langle T \rangle + T'_{RMS}$  and  $\langle T \rangle - T'_{RMS}$  and

	□	X
$c_{S1} (\langle T \rangle + T'_{RMS}) / \langle c_{S1} \rangle$	25%	24%
$c_{S1} (\langle T \rangle - T'_{RMS}) / \langle c_{S1} \rangle$	31%	31%

TABLE 1. Equilibrium mass fraction of species S1 evaluated at the maximum and minimum local temperatures in the boundary layer and relative to its mean.

normalized by  $\langle c_{S1} \rangle$  (which equals  $c_{S1}$  evaluated at  $\langle T \rangle$ ). We see that 5% fluctuation in the mean temperature can cause a 31% difference in the chemical composition. Clearly, the equilibrium composition is a very strong function of the temperature. This is reflected in the magnitude of  $c'_{S1}$  within the boundary layer, which is shown in Fig. 4b. We see that variations in the equilibrium mass fraction are nearly that produced by the temperature fluctuations.

### Turbulence-chemistry interaction

In this section we study the turbulence-chemistry interaction and the temperature fluctuation scaling by studying the budget of the terms in the evolution equations for the temperature variance and the turbulent kinetic energy. Figure 5 shows the effect of the source term on the temperature fluctuation variance. The symbols are shown for future reference. The source term has been decomposed into the forward and backward components,

$$\begin{aligned} w_{S1} &= -M_{S1} k_f \frac{\rho_{S1}}{M_{S1}} \left( \frac{\rho_{S1}}{M_{S1}} + \frac{\rho_{S2}}{M_{S2}} \right) \\ &\quad + M_{S1} k_b \frac{\rho_{S2}}{M_{S2}} \left( \frac{\rho_{S1}}{M_{S1}} + \frac{\rho_{S2}}{M_{S2}} \right) \quad (6) \\ &= w_f + w_b, \end{aligned}$$

where  $\rho_s$  and  $M_s$  are the density and molecular weight of species  $s$ ,  $k_f$  and  $k_b$  are the forward and backward reaction rates, respectively, and  $w_f$  and  $w_b$  represent the destruction and production of species S1. Thus,  $w_f$  reduces the magnitude of the temperature fluctuations as a result of endothermic reactions and  $w_b$  has the opposite effect. Figure 5 also shows that both exothermic and endothermic reactions take place within the boundary layer. Figure 6a shows the budget of  $\langle T'T' \rangle$  in the near wall region. At the wall the chemical production and thermal diffusion are balanced

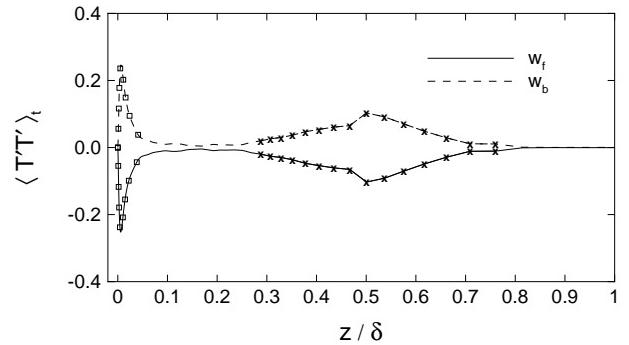


FIGURE 5. Contribution of the chemical production to  $\langle T'T' \rangle_t$ . The terms are normalized using  $u_\tau^3/cv z_\tau$ .

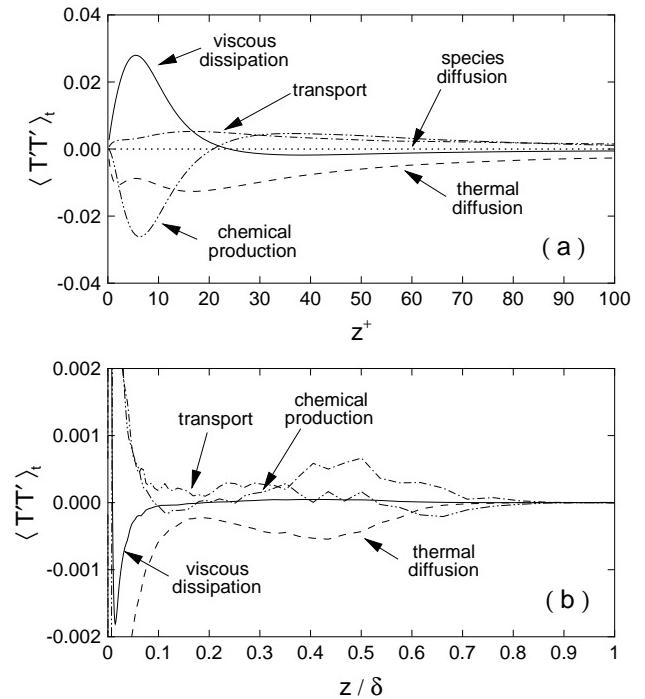


FIGURE 6. Budget of the terms in the evolution equation for  $\langle T'T' \rangle_t$  (a) near the wall and (b) across the boundary layer. The terms are normalized using  $u_\tau^3/cv z_\tau$ .

by the viscous dissipation and transport mechanisms. The species diffusivity is negligible since the gradients of species mass fraction are equal in magnitude and opposite in sign. Figure 6b shows the same budget throughout the entire boundary layer. The chemical production and transport mechanisms enhance the temperature fluctuations, however these terms are balanced by the thermal diffusion. The species diffusion term is negligible and not shown.

Figure 7a shows the budget of the turbulent kinetic energy in the near wall region. The turbulent kinetic energy is nearly in equilibrium. Figure 7b shows

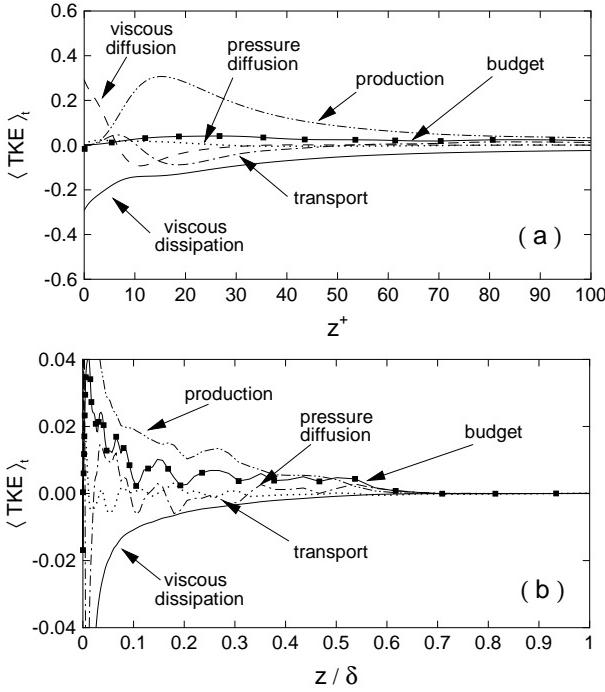


FIGURE 7. Budget of the terms in the evolution equation for  $\langle \bar{\rho} \bar{k} \rangle_t$  (a) near the wall and (b) across the boundary layer. The terms are normalized using  $\rho_w u_\tau^3 / z_\tau$ .

the same budget across the entire boundary layer. The production term is dominant causing a net production of turbulent kinetic energy. The production and transport terms have the same oscillatory behavior in  $0.1 \leq z/\delta \leq 0.3$ . This behavior is similar to that of the transport term in the equation for  $\langle T'T' \rangle_t$ , as shown in Fig. 6b. Figure 8a plots the temporal evolution of the friction velocity,  $u_\tau$ . After the initial transient, the oscillations in  $u_\tau$  indicate the presence of a physical mechanism that is damping and replenishing  $u_\tau$ . Figure 8b plots the turbulent kinetic energy across the boundary layer. Again the oscillatory behavior is observed in  $0.1 \leq z/\delta \leq 0.3$ , as in the transport and production mechanisms for the evolution of  $\langle T'T' \rangle_t$  and  $\langle TKE \rangle_t$ . As in isotropic turbulence,<sup>1</sup> this result suggests that a feedback mechanism between the turbulent motion and the chemical reactions takes place.

The effect of endothermic reactions is to damp the temperature fluctuations. However for the conditions chosen, the turbulent kinetic energy in the boundary layer is self-sustained. Therefore, the turbulent temperature fluctuations are maintained. The exothermic reactions, however, act as heat sources increasing the temperature fluctuations. Both endothermic and reactions cause localized compressions and

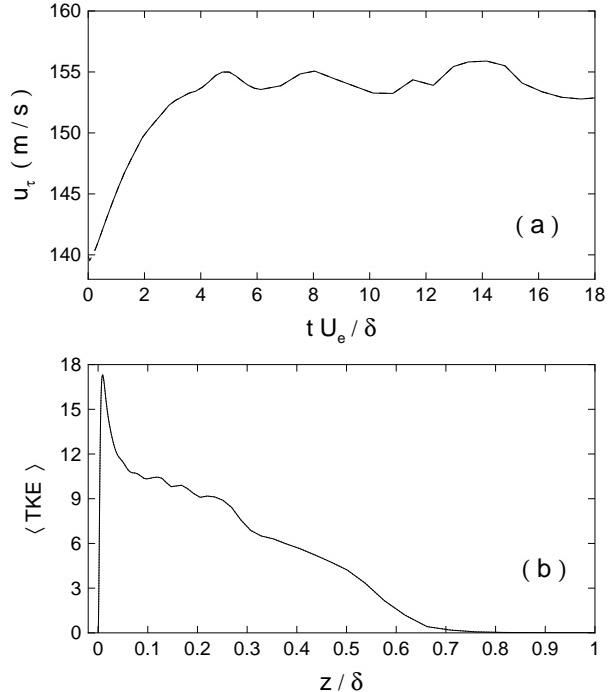


FIGURE 8. (a) Temporal evolution of the wall-friction velocity and (b) turbulent kinetic energy profile normalized using  $\rho_w u_\tau^2$ .

exothermic expansions within the boundary layer. The turbulent kinetic energy feeds from the thermal energy. The results suggest that this feedback mechanism takes place through the transport term in the equation for  $\langle T'T' \rangle_t$  and through the production and transport mechanisms in the equation for  $\langle TKE \rangle_t$ . The transport term for  $\langle T'T' \rangle_t$  includes the correlation between temperature fluctuations and dilatation, which explains the energy transfer between the turbulent kinetic energy and the internal energy through the chemically induced expansions and compressions.

Figure 9 plots the magnitude of the temperature fluctuations versus the heat ratio, eq. (2), in the viscous sublayer and near  $z/\delta = 0.5$ . (These boundary layer locations are marked with symbols in Fig. 5.) The data includes several time steps during the simulation. The power law relation between temperature fluctuations and the heat ratio resembles that found in isotropic turbulence. The data collapse very well in the viscous sublayer, where the turbulence scales are nearly isotropic. Near the boundary layer edge however, the agreement is not so good. This could be because near the boundary layer the numerical resolution is not as good, since the computational grid is exponentially stretched. This can be seen in the lower

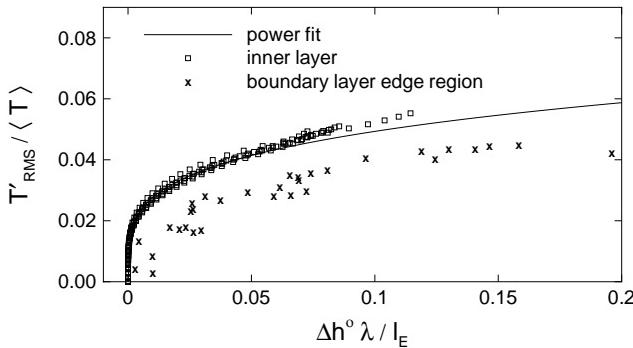


FIGURE 9. Temperature fluctuation versus heat ratio.

population of symbols for the data near the boundary layer. It is also possible that we have not gather sufficient statistics in time so as to get a large enough sample of data. A Reynolds number dependence is also possible, since the peak in the logarithmic region of the turbulent profiles is highly dependent on the Reynolds number. None of these reasons or others can be proven true with the small dataset that we are working with.

### Conclusions

In this paper, we have analyzed the direct numerical simulation database of a chemically reacting, turbulent boundary layer at Mach 4,  $Re_\theta = 7000$ , and isothermal wall-temperature condition. The budget of the terms in the evolution equation for the temperature show that the mean flow is in chemical equilibrium. However, the temperature fluctuations increase the reaction rates and therefore the chemistry is active throughout the boundary layer. The magnitude of the fluctuations in temperature and species mass fraction show that a 5% fluctuation in temperature can cause a 30% fluctuation in the species mass fraction. If the boundary layer is in chemical non-equilibrium, such large fluctuations in the species mass fraction may have a significant effect in the average composition of the gas and therefore in the heating rates to the wall. Additional simulations are required to verify this.

The evolution equation for the temperature fluctuations show that endothermic reactions reduce the temperature fluctuations, whereas exothermic reactions act as heat sources that increase  $T'_RMS$ . The budget of turbulent kinetic energy shows that the production and transport mechanisms are enhanced by the presence of reactions. The oscillations found in the evolution of the wall-friction velocity and in the profile of turbulent kinetic energy indicate the presence of a physical mechanism that is damping and replenishing the turbulent kinetic energy.

The effect of endothermic reactions is to damp the temperature fluctuations. However, the turbulent ki-

netic energy in the boundary layer is self-sustained. Therefore, the turbulent temperature fluctuations are maintained. As mentioned above, exothermic reactions increase the magnitude of the temperature fluctuations and the temperature fluctuations increase the reaction rates. Both endothermic and exothermic reactions cause localized compressions and expansions within the boundary layer that feed the turbulent kinetic energy. The results suggest that this feedback mechanism takes place through the transport term in the equation for  $\langle T'T' \rangle_t$  and through the production and transport mechanisms in the equation for  $\langle pk \rangle_t$ . The transport term for  $\langle T'T' \rangle_t$  includes the correlation between temperature fluctuations and dilatation, which explains the energy transfer between the turbulent kinetic energy and the internal energy through the chemically induced expansions and compressions. This result is consistent with that found using the DNS data of reacting isotropic turbulence<sup>1,2</sup> and with the theoretical work of Eschenroeder.<sup>5</sup>

Also as in isotropic turbulence, we find that the temperature variance can be expressed as  $A (\overline{\Delta h^o \lambda} / l_E)^B$ . Where  $\lambda / l_E$  is obtained from the nondimensional governing parameters and represents the ratio of the characteristic distance traveled by a fluid particle to the characteristic distance of acoustic radiation. Since  $\overline{\Delta h^o \lambda} / l_E$  is a mean flow quantity, it could potentially be used to predict the temperature fluctuations in Reynolds-averaged Navier-Stokes or large-eddy simulations. However, further testing of the scaling must be performed over a wider range of conditions.

### Acknowledgments

We would like to acknowledge the support from the NASA Ames Research Center. A portion of the computer time was provided by the Army High Performance Computing Research Center under the auspices of the Department of the Army, Army Research Laboratory cooperative agreement number DAAH04-95-2-0003 / contract number DAAH04-95-C-0008, the content of which does not necessarily reflect the position or the policy of the government, and no official endorsement should be inferred. This work was supported in part by the Air Force Office of Scientific Research under grant AF/F49620-01-1-0060.

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